STRATEGIES FOR DESIGNING HYDROGEN-STORING LIQUIDS TO MEET REQUIRED PHYSICAL, CHEMICAL AND THERMAL PROPERTIES

Philip G. Jessop, Yi Cui, Dominik Wechsler, Boyd Davis, Ralph Whitney

Dept. of Chemistry, Queen's University, Kingston, ON, Canada K7L 3N6

One major factor preventing widespread use of automotive fuel cells is the lack of a viable on-board method for hydrogen storage. While many methods have been proposed, organic hydrogen-storage liquids have the economic advantage that they could be distributed using existing infrastructure (gas stations). However, they need to be designed so that they: (1) are capable of facile, clean and reversible dehydrogenation; (2) have a low dehydrogenation enthalpy so that dehydrogenation is favored at as low a temperature as possible; (3) are liquid and nonvolatile from -40 ˚C to the dehydrogenation temperature; (4) have a hydrogen storage capacity > 6 wt% and 45 g H_2 per litre; and (5) are stable against decomposition at operating temperatures. This presentation will describe several strategies for the design of liquids that can meet these requirements and preliminary results of investigations of the validity of these strategies.

Design strategies to be discussed include:

a) use of heteroaromatic rings (pioneered by Pez)
b) addition of electron-donating substituents (see Figure below)
c) addition of conjugated unsaturated substituents
d) use of high-density liquids as hydrogen storage media
e) combination of exothermic and endothermic reactions for heat balance

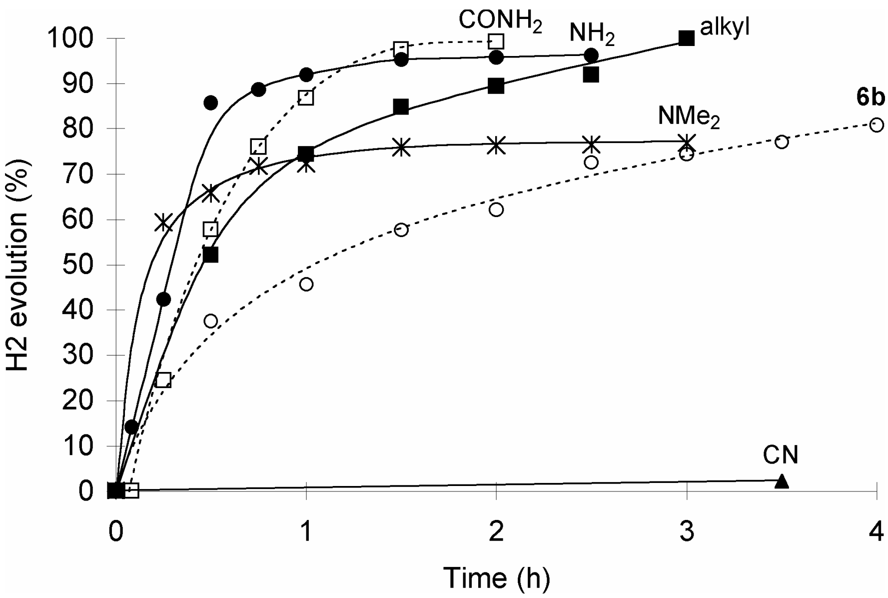

Figure. A comparison of the rates of hydrogen evolution of octahydro-1-methylindole and several piperidines over 5 % Pd/SiO_2 at 170 ˚C with constant but slow flow of N_2. The starting materials were 4-aminopiperidine, 4-dimethylaminopiperidine, piperidine-4-carboxamide, 4-cyanopiperidine, 1,3-di(piperidin-4-yl)propane, and 1-methyloctahydroindole (labelled **6b**).

Y. Cui, S. Kwok, A. Bucholtz, B. Davis, R. A. Whitney, P. G. Jessop, ***New J. Chem.*** (2008), *in press*